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STRESS STUDIES IN EFG

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"The JPL Flat Plate Solar Array Project is sponsored by the U.S. Department of Energy and forms part of the Solar Photovoltaic Conversion Program to initiate a major effort toward the development of flat plate solar arrays. This work was performed for the Jet Propulsion Laboratory, California Institute of Technology by agreement between NASA and DOE."

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ABSTRACT

A program to study stress generation mechanisms in silicon sheet growth was started at Mobil Solar on July 9, 1982. The purpose of the research is to define post-growth temperature profiles for the sheet that can minimize its stress during growth at high speeds, e.g., greater than 3 cm/min. The initial tasks described in this report concern work in progress toward the development of computing capabilities to (i) model stress-temperature relationships in steady-state ribbon growth, and (ii) provide a means to calculate realistic temperature fields in ribbon, given growth system component temperatures as boundary conditions. If it is determined that low stress configurations can be achieved, the modeling is to be tested experimentally by constructing low-stress growth systems for EFG silicon ribbon.

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I. INTRODUCTION

A satisfactory model that can account for stresses generated in silicon sheet grown at high speeds is not yet available. Numerous attempts to account for residual stresses have been made, but all of these suffer inadequacies in one area or another. The most prominent of these are the lack of a fully two-dimensional treatment of stress and temperature fields in the sheet width dimension, and the omission of plastic deformation effects. Two significant factors preventing the development of such a model have been the absence of adequate information on creep behavior of silicon at high temperatures that could be applicable to the sheet growth situation, and of experimental data on temperature fields and deformation modes of growing sheet that could guide the modeling effort.

This report describes the work in progress under this subcontract to attempt to develop and test in the laboratory a stress-temperature field model for EFG silicon ribbon that deals with the above deficiencies. In one subtask, a computer code to predict stress-temperature field relationships in steady-state sheet growth is being developed at Harvard University. The stress state will be parameterized by a two-dimensional temperature field and growth speed. Incorporation of time dependent stress relaxation effects through a creep law is also planned to model the impact of plastic flow on the sheet residual stress state. A second aspect of the program will deal with the development of a model to predict the temperature field in a moving sheet from

given system component temperatures (i.e., the sheet environment), and study experimental means to verify the model.

The goal of the program is to combine the results of these two areas of study to arrive at a model that can predict stress-temperature field relationships in steady-state silicon sheet growth under realistic conditions. Minimum stress configurations will be sought, and an attempt to construct an EFG silicon ribbon growth system that can verify this model will be made if it appears such configurations can be achieved experimentally. To aid the effort to correlate modeling results to experimental conditions, experimental means to examine temperature fields and stress generating process during growth are also under study.

II. PROGRESS REPORT

The first section that follows describes the strategy that has been adopted to develop a computer code to model the stress-temperature field relationship in a silicon sheet growing under steady-state conditions. This work is being done at Harvard University. The second section focuses on the development of a computer program to calculate ribbon temperatures for given temperature boundary conditions in an enclosure surrounding the ribbon, and to verify the calculation procedure experimentally. This part of the work is being done at Mobil Solar.

A. Stress Analysis of Steady-State Ribbon Growth (J.W. Hutchinson and J.C. Lambropoulos, Harvard University)

Work in the period July 9, 1982, to October 1, 1982, was largely directed towards developing a computer code for analyzing the stress distribution in a ribbon pulled from the melt through an arbitrary temperature field under steady-state conditions. The formulation of the problem and the numerical method for solving it are described below. Similar methods have been applied with success to analyze steady-state crack growth problems in elastic-plastic solids(1) and in elastic-creeping solids.(2)

The ribbon emerges from the melt at x = 0 and is pulled in the positive x-direction with uniform velocity V. It has width 2h extending from y = -h to y = h. The temperature distribution in the ribbon is denoted by T(x,y) and is assumed to be independent of time.

Plane stress conditions are assumed with non-zero stresses σ_{xx}, σ_{yy} and σ_{xy}. Steady-state conditions are assumed to exist so that the stresses, strain-rates and velocities are independent of time at any spatial point (but not, of course, for a material element). The additional velocity components are denoted by (v_x, v_y) so that the total velocity components are $(V + v_x, v_y)$, where the additional velocities are very small compared to the pull velocity V. The strain-rates are related to the velocities by

$$\dot{\varepsilon}_{ij} = \frac{1}{2}(v_{i,j} + v_{j,i}) \qquad (1)$$

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The material is taken to be an elastic-creeping solid. The numerical method is not tied to any particular form of the constitutive law. However, the law which looks most promising at the moment to represent existing creep and relaxation data for silicon has the form of the following prototype relation:

$$\dot{\varepsilon}_{ij} = \frac{1+\nu}{E}\dot{\sigma}_{ij} - \frac{\nu}{E}\dot{\sigma}_{kk}\delta_{ij} + \frac{3}{2}B\sigma_e^{\,n-1}s_{ij} + \alpha\dot{T}\delta_{ij} \tag{2}$$

Here, the dot denotes the time-rate of change with respect to a material element and, for steady-state pulling through a time-independent temperature distribution,

$$\dot{T} = V\,T_{,x} \tag{3}$$

The inelastic creep contribution is of the standard power-law form with s_{ij} as the stress deviator and $\sigma_e = (3s_{ij}s_{ij}/2)^{1/2}$ as the effective stress. This gives a creep-rate in uniaxial tension at a given temperature as $\dot{\varepsilon} = B(T)\sigma^n$, where B is a strong function of temperature. The coefficient of thermal expansion α is also a known function of temperature. The creep term in (2) characterizes secondary creep so that a primary creep contribution is not included in (2). In principle there would be no difficulty in including more accurate creep descriptions; however, available data for silicon does not appear to justify a more complicated description at this point. The data does permit specification of B(T) and α(T).

In addition to the above equations, the equations of in-plane equilibrium, $\dot{\sigma}_{ij,j} = 0$, must be specified. The equivalent variational equation of equilibrium is:

$$\int_A \dot{\sigma}_{ij}\delta v_{i,j}dA = 0 \tag{4}$$

and no boundary terms are involved since the tractions vanish everywhere on the boundary. Given the stress-rate field, the stress field is related to it by the steady-state relation

$$\dot{\sigma}_{ij} = V\,\sigma_{ij,x} \tag{5}$$

Since the stress is zero at the melt interface, (5) implies:

$$\sigma_{ij} = V^{-1}\int_o^x \dot{\sigma}_{ij}dx \tag{6}$$

This completes the set of governing equations.

The numerical method uses a velocity-based finite element method to discretize the fields. The problem is inherently nonlinear and therefore an iteration procedure is employed to obtain the solution. In principle, the iteration scheme works as follows.

1. At the end of any iteration an estimate of the stresses is available. This estimate is used to calculate an estimate of the creep strain-rates in each element for the next iteration.

2. The finite element method is used to obtain the next improved estimate of the velocity field. The method employs a variational equation where the creep-rate terms and the thermal strains both enter as body force terms.

3. Given the new estimate of the velocities, the new estimate of the total strain-rate is available and this is used in (2) to obtain a new estimate of the stress-rate.

4. Given the new estimate of the stress-rate, the new estimate of the stresses are obtained from (6). The steps in a

given iteration are now complete, and the next iteration can start over with step 1.

Iteration is continued until convergence is obtained. The above scheme is modified in several nonessential ways to improve efficiency and stability.

During the quarterly period starting from July 9, 1982, the existing computer code from the work in (1) and (2) was modified to be applicable to the ribbon growth problem. Efforts to check out the program on some trial elastic problems were started. These efforts will be continued into the next quarterly period, when we will also initiate calculations using realistic temperature distributions with creep deformations included.

B. Temperature Field Determination in Moving Silicon Sheet
(R.O. Bell and J.P. Kalejs, Mobil Solar)

In order to calculate the stress distribution and how it varies with growth speed in a solid, it is necessary to have a rather precise knowledge of the temperature distribution as a function of position and time. One possibility is that of measuring the temperature using thermocouples attached to the ribbon, but the large number of points required makes this experimentally impractical. Thus, we are left with the necessity of determining the temperature distribution by calculation and the use of experiment to validate the results by measuring a few selected points.

The calculations have been made in two steps. The first was to use the surrounding temperatures and geometry to calculate the heat flux arriving at the surface of the ribbon. This was done by

assuming the surrounding surfaces were black bodies and integrating view factors to calculate the flux.

The second step was to calculate the interaction of this flux with the silicon ribbon making use of the physical properties of the material. Silicon is not a black body, but rather a gray body that is semi-transparent for energies below its band gap. Thus, it is necessary to calculate all energy interchanges as a function of wavelength and integrate to obtain the total net radiation flux.

Some of the more important assumptions are the following.

1. For photon energies less than the band gap, silicon is semi-transparent, but for photon energies greater it is opaque.

2. Below the energy gap, the absorptivity and emissivity are determined by the free carrier absorption and are functions of wavelength. Since at high temperatures silicon is intrinsic, the carrier concentration depends only on temperature.

3. The emissivity above the energy gap is one minus the reflectivity. The reflectivity at all wavelengths is a function of the index of refraction and thus of wavelength.

4. The energy gap and thermal conductivity are functions of temperature.

5. The differential equation governing heat transport is that for a "thin" two-dimensional solid and is given by

$$\frac{d}{dz}\left(k\,\frac{dT}{dz}\right) + \frac{d}{dy}\left(k\,\frac{dT}{dy}\right) + vC_v\,\frac{dT}{dz} = \frac{2}{t}\,F(T,z,y)$$

where k is the thermal conductivity, v is the velocity in the z direction, C_v is the specific heat, t is the ribbon thickness and F(T,z,y), which is an integral over wavelength, is the difference in flux arriving and leaving the surface.

Needless to say, not much can be done analytically with such a highly non-linear equation and, unless properly chosen, even numerical techniques can be unsatisfactory. We have adapted a technique called "quasi-linearization" and have obtained convergence in a relatively few iterations.[3] This procedure is closely related to the Newton-Raphson method.

In order to produce a condition where experiment and theory could be compared, a highly idealized situation was constructed in ribbon growth Furnace 17. A long slot (large enough to accommodate a 5 cm wide ribbon about 25 cm in length) was milled in a block of fiberform insulation. Thermocouples were embedded in the walls to measure the surface temperature and two more thermocouples were attached to the ribbon. A plate at the bottom of the slot was heated to near the melting point of silicon and its temperature was monitored also. With the ribbon in the slot, and resting against the plate, thermocouple readings were taken. This was done for two different slot aspect ratios. Initial comparisons between calculations (in this case the ribbon velocity is zero) and experiment seemed to indicate that in the experiment the ribbon was 65°C too hot. This discrepancy was resolved when we determined that the thermocouples embedded in the walls were not recording the actual wall surface temperature because they were about 1 mm from the surface. They were low by about the right amount to explain the disagreement.

The second calculation has been to model the expected temperature near the center of a ribbon for a typical "cold shoe"

geometry. Figure 1 shows the geometry modeled. Die top radiation shield (not shown), cold shoe and linear cooling plate temperatures were all obtained experimentally from measurements using thermocouples embedded in the respective components. They thus define a ribbon environment with prescribed radiating enclosure wall temperatures. The linear cooling plate temperature profile is typical of that measured for power level settings used in growth of 10 cm wide ribbon. The cold shoe, which is at 450°C and 0.3 cm long, is located 0.2 cm above the die. We assume that all temperatures vary linearly with position between the positions at which they were measured. A ribbon of thickness of 300 μm centered in the 0.25 cm gap is considered. The unknown temperatures in the model represent the die-radiation shield gap (1500°C), the radiation shield-cold shoe gap (1100°C-800°C), and the cold shoe-linear cooling plate gap (700°C-1000°C). The sensitivity of the ribbon temperature profile to each of these temperature parameters, as well as to the enclosure size (ribbon to wall spacing) will be investigated in the future.

The calculations were made with the boundary conditions on the ribbon that at the die the temperature is that of melting silicon (1412°C) and at the exit to the furnace $dT/dz = 0$. We assume the horizontal flux is constant across the ribbon width and at the edges $dT/dy = 0$.

Figure 2 shows the ribbon temperature as a function of distance from the die. Also shown is the temperature of the environment. As expected, the temperature reaches a minimum

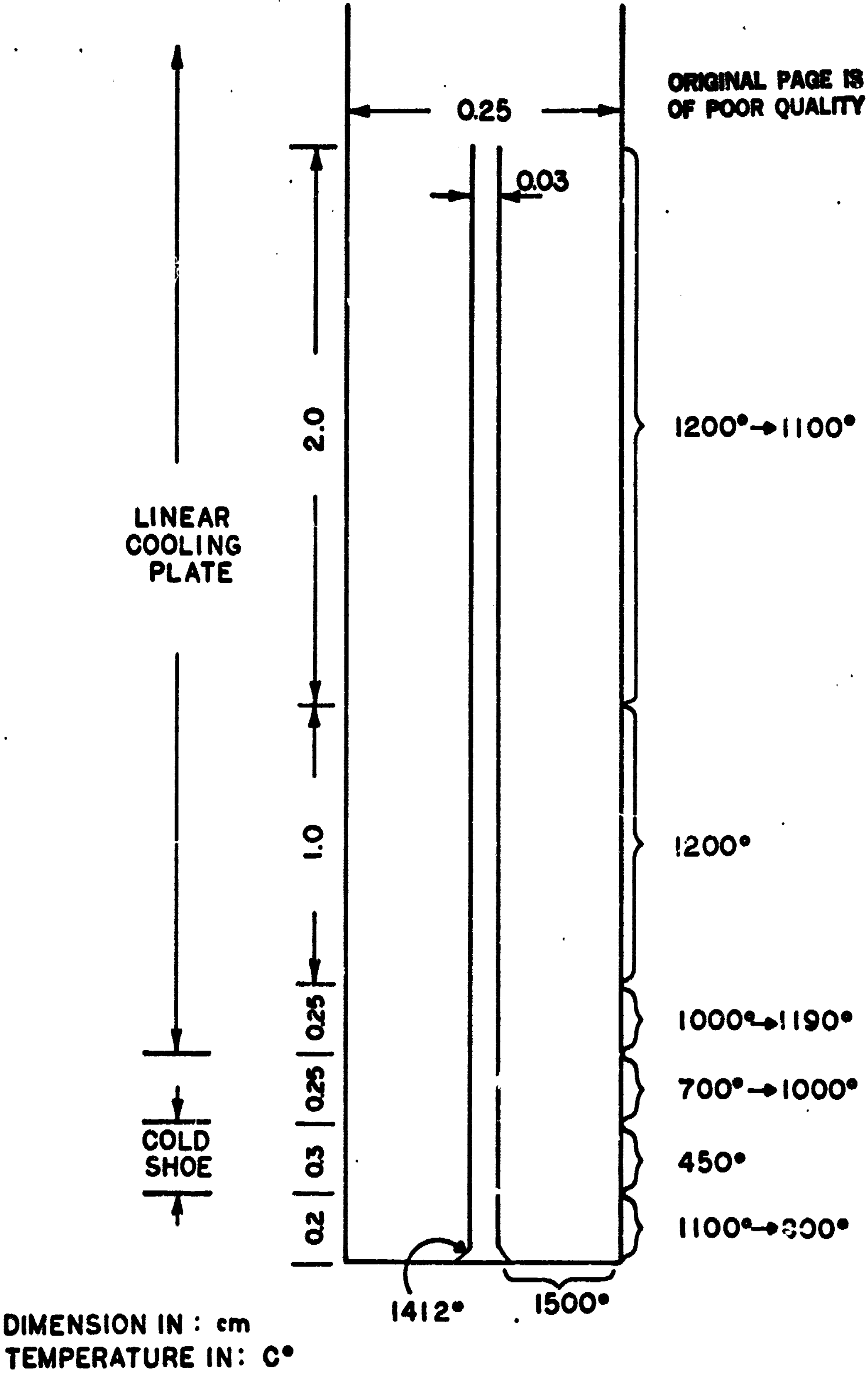

Fig. 1. "Cold shoe" geometry used to calculate the temperature distribution in ribbon.

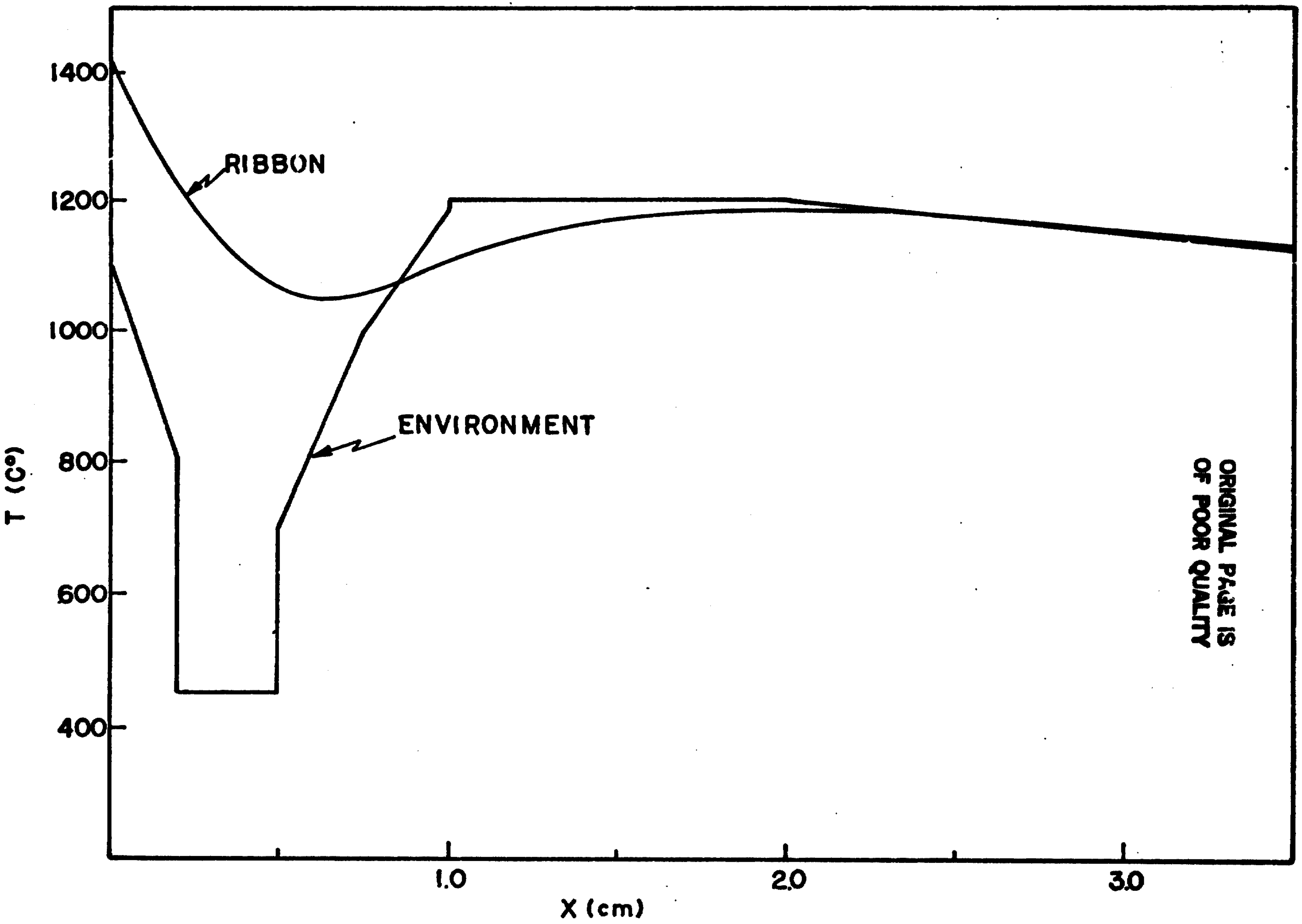

Fig. 2. Temperature distribution of the environment and in a 300 μm thick ribbon.

(1053°C) slightly above the cold shoe after which it increases to maximum (1188°C) in the afterheater. The gradient at the interface of 980°C/cm will support a growth rate of about 3 cm/min. This is lower than the demonstrated speed capability of the 10 cm wide ribbon system, which is estimated to be about 4 to 4.5 cm/min at this thickness ribbon. The sensitivity analysis planned for investigating the influence of the unknown temperatures parameterizing the system should be able to determine if this simplified model can predict the experimentally observed speed capability, while further refinement of the heat transfer model is also planned.

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APPENDIX

WORK BREAKDOWN STRUCTURE AND PROGRAM PLAN

July 9, 1982 - July 8, 1983

"STRESS STUDIES IN EFG"

SUBJECT	DESCRIPTION	JUL	AUG	SEP	OCT	NOV	DEC	'83 JAN	FEB	MAR	APR	MAY	JUN	JUL
Theoretical	Investigation of zero stress temperature profiles and development of ribbon buckle computational facility.	X	---	---	---	---	X							
	Development of computer program to calculate temperature profiles in ribbon.	X	---	---	---	---	X							
	Modeling of reduced stress growth configurations.						X	---	---	---	---	---	X	
Experimental	Development of temperature sensing methods using optical fibers.					X	---	X						
	Advanced system design concept testing.						X	---	---	---	---	---	X	
Program Management	Progress reports, etc.	X	---	---	---	---	---	---	---	---	---	---	X	